Multi-objective Bayesian optimization of stochastic experiments

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Assembly System Design

VCCM

Goal

Efficiently find optimal solutions with a minimal set of computer/physical experiments, and considering

- Multiple objectives
- Uncertainty in outputs
- Potential feasibility constraints (on inputs/outputs)

Motivation

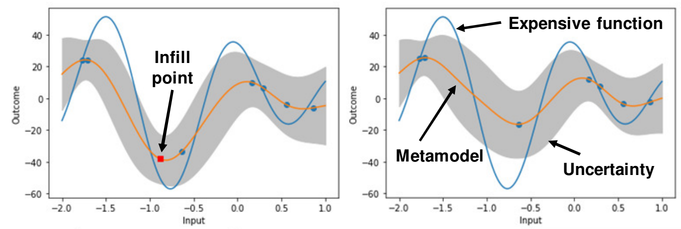
- In many real-life systems (engineering design, process design, supply chain design, etc.), the optimization problems studied are **multi-objective** (exhibiting *trade-offs* between individual objectives)**,** and outputs observations are **noisy** (repeated experiments of the same inputs may yield different output observations).
- The input/output relationships for objectives and constraints are often **black box: experimentation** is required to evaluate them. These (physical or computer) experiments can be **expensive (in terms of cost, time, etc),** and the budget for experimentation is typically constrained.
- The goal then is to detect solutions with very high quality (optimal or near-optimal) **within as few experiments as possible**.
- Traditional optimization heuristics (genetic algorithms, evolutionary algorithms) **are ill-suited** to achieve this goal.
- **Solution: Machine learning (ML)** techniques (fit for use in settings with scarce data), combined with **optimization (OR)** insights and/or **statistical learning**

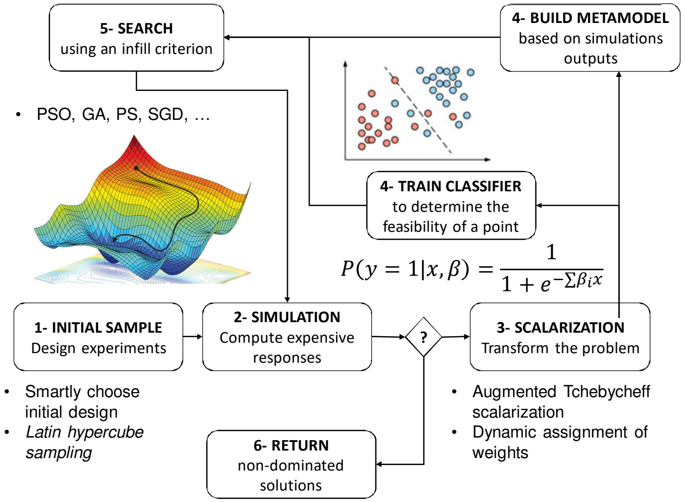
Approach

- Model (expensive, black-box) continuous output functions *f* using **Gaussian Process Regression (GPR)** with heterogeneous noise (**stochastic kriging**) [1]. This allows us to obtain an estimation of the output value **($\hat{f}$)** at unobserved locations, along with an estimator for the **uncertainty** on this value (s^2, also referred to as the MSE). This MSE captures both **metamodel uncertainty** and **stochastic uncertainty**.
- Use **infill criterion (acquisition function)** to select next input combination to sample (**Bayesian optimization**) .

Infill criterion [2]

$$CMEI = \left[(\hat{f}_{min} - \hat{f})\Phi\left(\frac{\hat{f}_{min} - \hat{f}}{s}\right) + s\phi\left(\frac{\hat{f}_{min} - \hat{f}}{s}\right)\right] * P(y = 1|x, \beta)$$





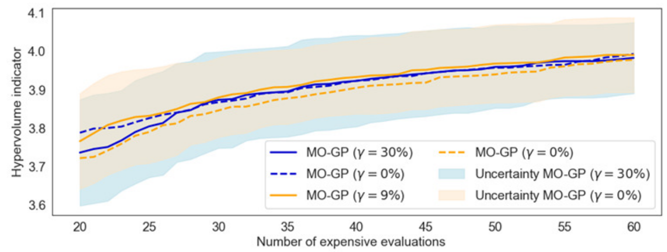
*Algorithm based on the work presented in [3]

Results

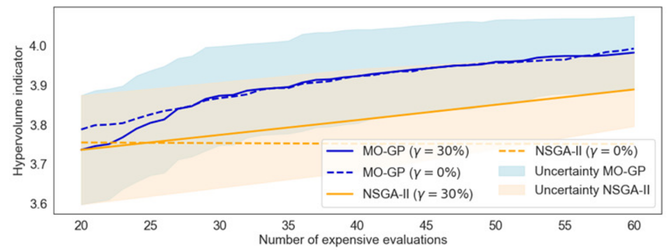
Parameter optimization for plasma process in adhesive bonding application (JMLab, Flanders Make)

- Maximize break strength and minimize production costs (bi-objective) by tuning 6 parameters
- Avoid configurations that lead to adhesive failure or visual damage of the sample

Results MO-GP for low and moderate noise levels (γ)



Outperforms common evolutionary algorithms (NSGA-II)



Key take-aways

- Efficient and effective search for solutions to expensive optimization problems with noise
- Proposed (Bayesian) approach is shown to be robust to the noise level and clearly outperforms the well-known NSGA-II

Further reading

[1] https://doi.org/10.1287/opre.1090.0754
[2] https://doi.org/10.1080/0740817X.2012.706377
[3] https://doi.org/10.1016/j.ejor.2019.12.014